THE INVENTION CLAIMED IS

1. A method of finding 3D similarities in protein the structure of a first molecule and of a second molecule, comprising the steps of:

processing preselected structure information of alignment of residue-residue correspondence,

comparing the first molecule and the second molecule using said preselected information and using Longest Continuous Segments (LCS) analysis,

comparing the first molecule and the second molecule using said preselected information and using Global Distance Test (GDT) analysis,

comparing the first molecule and the second molecule using said preselected information and using Local Global Alignment Scoring function (LGA_S) analysis,

repeating said steps to find all the regions of 3D similarities between considered protein structures, and

generating an output containing complete information about the quality of the calculated alignment.

2. The method of finding 3D similarities in protein structures of claim 1 wherein said Longest Continuous Segment (LCS) analysis is performed to detect for each consecutive residue from the first molecule the longest continuous regions of residue pairs that can fit under selected RMSD cutoff.

3. The method of finding 3D similarities in protein structures of claim 1 wherein said Global Distance Test (GDT) analysis comprises the following steps, (a) initiate an alignment, (b) verify (modify) an alignment and apply the transform, (c) identify all atom pairs for which the distance is larger than the threshold, (d) re-obtain the transform, excluding those atoms, (e) repeat steps (b)

– (d) until the set of atoms used in calculations is the largest and the same for two cycles running.

4. The method of finding 3D similarities in protein structures of claim 1 wherein said preselected structure information regarding the first molecule and said preselected information regarding the second molecule do not have significant amino acid sequence similarity.

5. The method of finding 3D similarities in protein structures of claim 1 wherein said step of comparing the first molecule and the second molecule using said preselected information and said Longest Continuous Segment (LCS) analysis, and said Global Distance Test (GDT) analysis, and said step of comparing the first molecule and the second molecule using said preselected information and said Local Global Alignment Scoring function (LGA_S) analysis provides data that can be used to analyze the correspondence between structure alignment and sequence alignment.

6. The method of finding 3D similarities in protein structures of claim 5 wherein the format of the output results from the LGA_5 analysis provides the complete information about the quality of the calculated alignment (distances between the corresponding residues, LCS data and GDT data). The designed format of the output data allows reporting the comprehensive information about the regions of local and global similarities between analyzed protein structures (Molecule-1 and Molecule-2).

7. A method of finding 3D similarities in protein the structure of a first molecule (Molecule-1) and of a second molecule (Molecule-2), comprising the steps of:

analyzing a preselected structure alignment (residue-residue correspondence),

comparing the first molecule and the second molecule using said preselected information and Longest Continuous Segments (LCS) analysis,

comparing the first molecule and the second molecule using said preselected information and Global Distance Test (GDT) analysis,

comparing the first molecule and the second molecule using said preselected information and Local Global Alignment Scoring function (LGA_S) analysis,

repeating said steps to find all the regions of 3D similarities between considered protein structures, and finally

generating the output from the program containing the complete information about the quality of the calculated alignment (distances between the corresponding residues, LCS data and GDT data).

8. The method of finding 3D similarities in protein structures of claim 7 wherein said Longest Continuous Segment (LCS) analysis is performed to detect for each consecutive residue from the molecule-2 the longest continuous regions of residue pairs that can fit under selected RMSD cutoff.

9. The method of finding 3D similarities in protein structures of claim 7 wherein said Global Distance Test (GDT) analysis comprises the following steps, (a) initiate an alignment, (b) verify (modify) an alignment and apply the transform, (c) identify all atom pairs for which the distance is larger than the threshold, (d) re-obtain the transform, excluding those atoms, (e) repeat steps (b) – (d) until the set of atoms used in calculations is the largest and the same for two cycles running.

10. The method of finding 3D similarities in protein structures of claim 7 wherein said preselected information regarding the first molecule and said

preselected information regarding the second molecule do not have significant amino acid sequence similarity.

11. The method of finding 3D similarities in protein structures of claim 7 wherein said step of comparing the first molecule and the second molecule using said preselected information and Longest Continuous Segment (LCS) analysis, and Global Distance Test (GDT) analysis, and said step of comparing the first molecule and the second molecule using said preselected information and Local Global Alignment Scoring function (LGA_S) analysis provides data that can be used to analyze the correspondence between structure alignment (structure similarity) and sequence alignment (sequence similarity).

12. The method of finding 3D similarities in protein structures of claim 7 wherein the format of the output results from said LGA analysis provides complete information about the quality of the calculated alignment (distances between the corresponding residues, LCS data and GDT data).

13. The method of finding 3D similarities in protein structures of claim 7 wherein the designed format of the output data allows reporting of the comprehensive information about the regions of local and global similarities between analyzed protein structures of Molecule-1 and Molecule-2.